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                 FSTA enhanced with new thesaurus edition
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         AUG 13
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                 CA/CAplus enhanced with CAS indexing in pre-1907 records
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                 USPATOLD now available on STN
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                 spectral property data
                 STN AnaVist, Version 2.0, now available with Derwent
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         SEP 13
         SEP 13
                 INPADOCDB enhanced with monthly SDI frequency
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                 CA/CAplus enhanced with printed CA page images from
         SEP 17
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                 CA/CAplus enhanced with pre-1907 records from Chemisches
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                 Derwent Indian patent publication number format enhanced
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         NOV 19
                 WPIX enhanced with XML display format
NEWS 19
         NOV 30
                 ICSD reloaded with enhancements
NEWS 20
         DEC 04
                 LINPADOCDB now available on STN
NEWS 21
         DEC 14
                 BEILSTEIN pricing structure to change
NEWS 22
         DEC. 17
                 USPATOLD added to additional database clusters
NEWS 23
         DEC 17
                 IMSDRUGCONF removed from database clusters and STN
NEWS 24
         DEC 17
                 DGENE now includes more than 10 million sequences
NEWS 25
         DEC 17
                 TOXCENTER enhanced with 2008 MeSH vocabulary in
                 MEDLINE segment
NEWS 26
         DEC 17
                 MEDLINE and LMEDLINE updated with 2008 MeSH vocabulary
         DEC 17
                 CA/CAplus enhanced with new custom IPC display formats
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NEWS 28
         DEC 17
                 STN Viewer enhanced with full-text patent content
                 from USPATOLD
                 STN pricing information for 2008 now available
NEWS 29
         JAN 02
NEWS 30
         JAN 16
                 CAS patent coverage enhanced to include exemplified
                 prophetic substances
NEWS EXPRESS
              19 SEPTEMBER 2007: CURRENT WINDOWS VERSION IS V8.2,
              CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
              AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.
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=> file registry

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COST IN U.S. DOLLARS
FULL ESTIMATED COST

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TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

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Uploading C:\Documents and Settings\jcho2\My Documents\10542914.str

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

Structure attributes must be viewed using STN Express query preparation.

=> s 11 exa full FULL SEARCH INITIATED 19:45:47 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 3 TO ITERATE

100.0% PROCESSED 3 ITERATIONS 1 ANSWERS SEARCH TIME: 00.00.01

=> file caplus
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 60.77 60.98

FULL ESTIMATED COST

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FILE COVERS 1907 - 22 Jan 2008 VOL 148 ISS 4 FILE LAST UPDATED: 21 Jan 2008 (20080121/ED)

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=> s 12

1 L2

=> d 13 bib abs hitstr

- L3 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN
- AN 2004:633495 CAPLUS
- DN 141:151034
- TI Use of a composition comprising vitamin K1 oxide or a derivative thereof for the treatment and/or the prevention of mammalian dermatological lesions
- IN Marchal, Alfred
- PA Auriga International S.A., Belg.
- SO PCT Int. Appl., 17 pp. CODEN: PIXXD2
- DT Patent
- LA English
- FAN.CNT 2

FAN.																		
	PAT	CENT :	NO.			KIN	D	DATE			APPL	ICAT:	ION !	NO.		Di	ATE	
							-				<b>-</b> -							<b>-</b>
ΡI	WO 2004064798			A1 20040805			WO 2004-BE11					20040120						
		W:	ΑE,	AG,	AL,	AM,	AT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	ΒZ,	CA,	CH,
								DE,										
			GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	ΚP,	KR,	ΚZ,	LC,
								LV,										
	EΡ	1442	738			A1		2004	0804		EP 2	003-	4470	19		2	0030	128
		R:						ES,										PT,
								RO,										
		2513						2004										
	ΕP	1594	456			<b>A</b> 1		2005	1116		EP 2	004-	7033	19		2	0040	120
		R:						ES,										
			ΙE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL,	TR,	ВG,	CZ,	EE,	ΗU,	SK	
	CN	1738	594			Α		2006	0222		CN 2	004-	8000	2490		2	0040	120

		JP 2006515873	T	20060608	JP 2006-500422	20040120
		US 2006154983	A1	20060713	US 2005-542914	20050720
	PRAI	IN 2005DN03209	Α	20070413	IN 2005-DN3209	20050720
		US 2003-319887P	P	20030120		
		EP 2003-447019	Α	20030128		
	US 2002-361234P	P	20020301			
		WO 2004-BE11	W	20040120		
	os	MARPAT 141:151034				

The invention discloses the use of a composition which comprises an adequate pharmaceutical or cosmetic carrier or diluent and a sufficient amount of vitamin K1 oxide, or a derivative thereof, for the treatment and/or the prevention of mammalian dermatol. lesions. The invention also discloses a cosmetic composition which comprises an adequate cosmetic carrier, phospholipids and vitamin K1 oxide or derivative thereof.

TT 729596-39-8

729596-39-8
RL: COS (Cosmetic use); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(vitamin K1 oxide or derivative for treatment and/or prevention of dermatol. lesions)

RN 729596-39-8 CAPLUS

CN Naphth[2,3-b]oxirene-2,7-dione, la,7a-dihydro-la-methyl-7a-(3,7,11-trimethyl-2-dodecenyl)- (9CI) (CA INDEX NAME)

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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STRUCTURE FILE UPDATES: 21 JAN 2008 HIGHEST RN 1000370-19-3 DICTIONARY FILE UPDATES: 21 JAN 2008 HIGHEST RN 1000370-19-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

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http://www.cas.org/support/stngen/stndoc/properties.html

=>

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STRUCTURE UPLOADED L4

=> d 14

L4 HAS NO ANSWERS

L4STR

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

Structure attributes must be viewed using STN Express query preparation.

=> s 14 sss sam

SAMPLE SEARCH INITIATED 19:48:44 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED -19 TO ITERATE

O ANSWERS 19 ITERATIONS 100.0% PROCESSED

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

119 TO 641 PROJECTED ITERATIONS:

0 0 TO PROJECTED ANSWERS:

0 SEA SSS SAM L4 L5

=> s 14 sss full

FULL SEARCH INITIATED 19:48:51 FILE 'REGISTRY' 366 TO ITERATE

FULL SCREEN SEARCH COMPLETED -

1 ANSWERS 366 ITERATIONS 100.0% PROCESSED

SEARCH TIME: 00.00.01

1 SEA SSS FUL L4 1.6

=> d scan

1 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN L6

Naphth[2,3-b]oxirene-2,7-dione, la,7a-dihydro-la-methyl-7a-(3,7,11-IN

trimethyl-2-dodecenyl)- (9CI)

C26 H36 O3 MF

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

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L7 STRUCTURE UPLOADED

=> d 17 L7 HAS NO ANSWERS L7 STR

Structure attributes must be viewed using STN Express query preparation.

=> s 17 sss sam

SAMPLE SEARCH INITIATED 19:50:57 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 48 TO ITERATE

100.0% PROCESSED

48 ITERATIONS

O ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 545 TO 1375
PROJECTED ANSWERS: 0 TO 0

L8 0 SEA SSS SAM L7

=> s 17 sss full FULL SEARCH INITIATED 19:51:04 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 1250 TO ITERATE

100.0% PROCESSED 1250 ITERATIONS

25 ANSWERS

SEARCH TIME: 00.00.01

L9 25 SEA SSS FUL L7

=> d scan

L9 25 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN Naphth[2,3-b]oxirene-2,7-dione, 1a,7a-dihydro-1a-methyl-7a-(3,7,11-a)

trimethyl-2,6,10-dodecatrienyl)- (9CI)

MF C26 H32 O3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):5

L9 25 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN Naphth[2,3-b]oxirene-2,7-dione, la,7a-dihydro-la-methyl-7a-(3-methyl-2-butenyl)-, (laS)- (9CI)

MF C16 H16 O3

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L9 25 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN Naphth[2,3-b]oxirene-2,7-dione, la,7a-dihydro-la-methyl-7a-(3-methyl-2-butenyl)- (9CI)

MF C16 H16 O3

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L9 25 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN Naphth[2,3-b]oxirene-2,7-dione, 1a,7a-dihydro-1a-methyl-7a-(3,7,11,15-tetramethyl-2-hexadecenyl)-, [1aS-[1a $\alpha$ ,7a $\alpha$ (2E,7S\*,11S\*)]]- (9CI)

MF C31 H46 O3

Absolute stereochemistry. Double bond geometry as shown.

$$\begin{array}{c} \text{Me} \\ \text{CH}_2)_{\overline{3}} \\ \text{R} \\ \text{CH}_2)_{\overline{3}} \\ \text{R} \\ \text{CH}_2)_{\overline{3}} \\ \text{CHMe}_2 \\ \text{Me} \\ \text{O} \\ \text{Me} \\ \text{O} \\ \text{Ne} \\ \text{O} \\ \text{CH}_2)_{\overline{3}} \\ \text{CHMe}_2 \\ \text{CH}_2)_{\overline{3}} \\ \text{CH}_3 \\ \text{CH}_4 \\ \text{CH}_2)_{\overline{3}} \\ \text{CH}_4 \\ \text{CH}_2)_{\overline{3}} \\ \text{CH}_4 \\ \text{CH}_2)_{\overline{3}} \\ \text{CH}_5 \\ \text{CH}_6 \\ \text{CH}_7 \\ \text{CH$$

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L9 25 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN Naphth[2,3-b]oxirene-2,7-dione, 1a-[3,7,11,15,19,23-hexamethyl-25-(2,6,6-trimethyl-2-cyclohexen-1-yl)-2,10,14,18,22-pentacosapentaenyl]-1a,7a-dihydro-7a-methyl- (9CI)

MF C51 H74 O3

FILE COVERS 1907 - 22 Jan 2008 VOL 148 ISS 4 FILE LAST UPDATED: 21 Jan 2008 (20080121/ED) Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at: http://www.cas.org/infopolicy.html L16 180 L15 => s composition 714220 COMPOSITION 326493 COMPOSITIONS 1033254 COMPOSITION (COMPOSITION OR COMPOSITIONS) 1511686 COMPN 609718 COMPNS 1851288 COMPN (COMPN OR COMPNS) L17 2329674 COMPOSITION (COMPOSITION OR COMPN) => s 116 and 117 26 L16 AND L17 => d 118 1-26 bib abs hitstr L18 ANSWER 1 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN 2005:369133 CAPLUS AN DN 142:435774 Compositions treatment of chronic inflammatory diseases TΙ ΙN Shapiro, Howard K. PA USA U.S. Pat. Appl. Publ., 44 pp., Cont.-in-part of U.S. Ser. No. 610,073, SO abandoned. CODEN: USXXCO DT Patent English FAN.CNT 4 KIND DATE APPLICATION NO. DATE PATENT NO. \_\_\_\_\_ -----\_\_\_\_\_ A1 20050428 US 2004-924945 20040824 B2 19920630 US 2005090553 PRAI US 1992-906909 US 1994-241603 B2 19940511 US 1997-814291 B2 19970310 B2 20000705 US 2000-610073 OS MARPAT 142:435774 This invention defines novel compns. that can be used for clin. treatment of a class of chronic inflammatory diseases. Increased generation of carbonyl substances, aldehydes and ketones, occurs at sites of chronic inflammation and is common to the etiologies of all of the clin. disorders addressed herein. Such carbonyl substances are cytotoxic and addnl. serve to perpetuate and disseminate the inflammatory process. This invention defines use of compns., the orally administered required primary agents of which are primary amine derivs. of benzoic acid capable of reacting with the carbonyl substances. P-Aminobenzoic acid (or PABA) is an example of the required primary agent of the present invention. PABA has a small mol. weight, is water soluble, has a primary amine group which reacts with carbonyl-containing substances and is tolerated by the body in relatively high dosages for extended periods. The method of the

present invention includes administration of a compn.

medicament co-agent recognized as effective to treat a chronic

comprising: (1) an orally consumed primary agent; (2) a previously known

inflammatory disease addressed herein administered to the mammalian subject via the oral route, other systemic routes of administration or via the topical route; and (3) optionally 1 or more addnl. orally consumed co-agent selected from the group consisting of antioxidants, vitamins, metabolites at risk of depletion, sulfhydryl co-agents, co-agents which may facilitate glutathione activity and nonabsorbable primary amine polymeric co-agents, so as to produce an additive or synergistic physiol. effect of an anti-inflammatory nature.

25486-55-9, Vitamin K1 oxide IT

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (compns. treatment of chronic inflammatory diseases)

RN 25486-55-9 CAPLUS

Naphth[2,3-b]oxirene-2,7-dione, 1a,7a-dihydro-la-methyl-7a-(3,7,11,15-CN tetramethyl-2-hexadecen-1-yl)- (CA INDEX NAME)

ANSWER 2 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2004:633495 CAPLUS

DN 141:151034

Use of a composition comprising vitamin K1 oxide or a derivative ΤI thereof for the treatment and/or the prevention of mammalian dermatological lesions

Marchal, Alfred ΙN

Auriga International S.A., Belg. PA

SO PCT Int. Appl., 17 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.	CNT 2																
	PATENT	NO.			KIN	D	DATE				ICAT				D.	ATE	
PI	WO 2004	10647	98		A1		2004	0805							2	0040	120
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	ΒB,	ВG,	BR,	BW,	BY,	ΒZ,	CA,	CH,
											EC,						
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KΕ,	KG,	KΡ,	KR,	ΚZ,	LC,
											MK,						
	EP 1442	2738			A1		2004	0804		EP 2	003-	4470	19		2	0030	128
	R:	AT,															
											TR,						
	CA 2513																
	EP 1594																
	R:	AT,															
											TR,						
	CN 1738																
	JP 2006	651581	73		$\mathbf{T}$						2006-						
	US 2006	61549	83		A1						2005-						
	IN 2009									IN 2	2005-	DN32	09		2	0050	720
PRAI	US 2003	3-319	887P		P		2003	0120									
	EP 2003						2003										
	US 2002	2-361	234P		P		2002	0301									
	WO 2004	4-BE1	1		W		2004	0120									
OS	MARPAT	141:	1510	34													

AB The invention discloses the use of a compn. which comprises an adequate pharmaceutical or cosmetic carrier or diluent and a sufficient amount of vitamin K1 oxide, or a derivative thereof, for the treatment and/or the prevention of mammalian dermatol. lesions. The invention also discloses a cosmetic compn. which comprises an adequate cosmetic carrier, phospholipids and vitamin K1 oxide or derivative thereof.

IT 25486-55-9, Vitamin K1 oxide RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(vitamin K1 oxide or derivative for treatment and/or prevention of dermatol. lesions)

RN 25486-55-9 CAPLUS

CN Naphth[2,3-b]oxirene-2,7-dione, 1a,7a-dihydro-la-methyl-7a-(3,7,11,15-tetramethyl-2-hexadecen-1-yl)- (CA INDEX NAME)

# RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 3 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2002:667430 CAPLUS

DN 137:195570

TI Methods of treating chronic inflammatory diseases using carbonyl trapping agents

IN Shapiro, Howard K.

PA USA

SO U.S., 23 pp., Cont.-in-part of U.S. Ser. No. 473,786, abandoned. CODEN: USXXAM

DT Patent

LA English

FAN.CNT 4

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
US 6444221	B1	20020903	US 1999-416120	19991012		
US 1992-906909	В2	19920630				
US 1995-473786	В2	19950607				
	PATENT NO US 6444221 US 1992-906909	PATENT NO. KIND US 6444221 B1 US 1992-906909 B2	PATENT NO. KIND DATE	PATENT NO. KIND DATE APPLICATION NO.  US 6444221 B1 20020903 US 1999-416120 US 1992-906909 B2 19920630		

OS MARPAT 137:195570 These and other objects of this invention are achieved by providing a novel method and compns. for the clin. treatment of chronic inflammatory diseases. This invention involves use of systemically administered compns. which include primary amine derivs. of benzoic acid as carbonyl trapping agents. These primary therapeutic agents act by chemical binding to and sequestering the aldehyde and/or ketone products of lipid peroxidn. Increased levels of lipid peroxidn. have been repeatedly demonstrated as a part of the non-enzymic "inflammatory cascade" process which underlies the secondary etiol. of chronic inflammatory diseases. P-Aminobenzoic acid (or PABA) is an example of the primary therapeutic agent of the present invention. PABA has a small mol. weight, is water soluble, has a primary amine group that reacts with carbonyl-containing metabolites under physiol. conditions and is tolerated by the body in relatively high dosages and for extended periods. The carbonyl sequestering agents are used in combination with at least one co-agent to produce an addnl. beneficial physiol. effect of an

anti-inflammatory nature. Such compns. are administered systemically entirely via the oral route. Co-agents of the present invention include anti-oxidants and free radical trapping compds. (e.g.,  $\alpha\text{-tocopherol})$ , compds. having indirect anti-oxidant activity (e.g., selenium), vitamins (e.g., pyridoxine HCl), compds. which facilitate kidney drug elimination (e.g., glycine), metabolites at risk of depletion (e.g., pantothenic acid), sulfhydryl containing chems. (e.g., methionine), compds. which facilitate glutathione activity (e.g., N-acetylcysteine), and non-absorbable polyamine co-agents (e.g., chitosan).

IT 25486-55-9, Vitamin K1 oxide

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(methods of treating chronic inflammatory diseases using primary amine derivs. of benzoic acid as carbonyl trapping agents and combination with other agents)

RN 25486-55-9 CAPLUS

CN Naphth[2,3-b]oxirene-2,7-dione, 1a,7a-dihydro-1a-methyl-7a-(3,7,11,15-tetramethyl-2-hexadecen-1-yl)- (CA INDEX NAME)

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 4 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1993:516157 CAPLUS

DN 119:116157

TI Hepatic concentration of vitamin K active compounds after application of phylloquinone to chickens on a vitamin K deficient or adequate diet

AU Guillaumont, M.; Weiser, H.; Sann, L.; Vignal, B.; Leclercq, M.; Frederich, A.

CS Inst. Pasteur Lyon, UFR Alexis Carrel, Lyon, 69372, Fr.

SO International Journal for Vitamin and Nutrition Research (1992), 62(1), 15-20

CODEN: IJVNAP; ISSN: 0300-9831

DT Journal

LA English

Liver and serum concns. of vitamin K active compds. were measured in two groups of (deficient and normal) broilers after i.v. administration of phylloquinone (1 mg/kg). Assays were performed by HPLC after extraction and purification of these compds. The only menaquinone found in the chicken was menaquinone-4. In the deficient group, the chickens exhibited hepatic concns. of vitamin K1, vitamin K1 epoxide and menaquinone-4 markedly lower than those of the control group. After administration of phylloquinone, vitamin K and vitamin K epoxide levels fell sharply. There is no hepatic storage of vitamin K comparable to that of vitamin A. However, while menaquinone levels were found to be stable in the control group, they rose significantly in the deficient group after vitamin K injection. The question is: is there a transformation of vitamin K into menaquinone and/or is there a preferential utilization of one of the vitamin K active compds.

IT 25486-55-9, Vitamin K1 epoxide RL: BIOL (Biological study)

(of blood serum and liver of chickens, i.v. phylloquinone effect on)

RN 25486-55-9 CAPLUS

CN Naphth[2,3-b]oxirene-2,7-dione, 1a,7a-dihydro-1a-methyl-7a-(3,7,11,15-tetramethyl-2-hexadecen-1-yl)- (CA INDEX NAME)

L18 ANSWER 5 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1991:629077 CAPLUS

DN 115:229077

TI Vitamin K epoxide reduction and vitamin K quinone reduction, gamma-carboxyglutamic acid analysis, and vitamin K-dependent activities from liver mitochondria and adipose tissue

AU Smalley, David Michael

CS Univ. Akron, Akron, OH, USA

SO (1991) 167 pp. Avail.: Univ. Microfilms Int., Order No. DA9115472 From: Diss. Abstr. Int. B 1991, 52(1), 222-23

DT Dissertation

LA English

AB Unavailable

IT 25486-55-9, Vitamin K epoxide
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of, by liver, adipose tissue in relation to)

RN 25486-55-9 CAPLUS

CN Naphth[2,3-b]oxirene-2,7-dione, 1a,7a-dihydro-1a-methyl-7a-(3,7,11,15-tetramethyl-2-hexadecen-1-yl)- (CA INDEX NAME)

L18 ANSWER 6 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1991:1894 CAPLUS

DN 114:1894

TI Vitamin K-dependent carboxylase: inhibitory action of polychlorinated phenols

AU Grossman, Carol P.; Suttie, J. W.

CS Coll. Agric. Life Sci., Univ. Wisconsin, Madison, WI, 53706, USA

SO Biochemical Pharmacology (1990), 40(6), 1351-5

CODEN: BCPCA6; ISSN: 0006-2952

DT Journal

LA English

AB A series of chlorinated phenols was assayed for their abilities to inhibit carboxylase in vitro. One compound, 2,3,5,6-tetrachlorophenol, was as potent a carboxylase inhibitor as 2,3,5,6-tetrachloropyridinol (TCP) (I50

= 5-10  $\mu$ M). Four compds. with substituents in the 4 position exhibited I50 5-20 times greater than the identical structures with H in the 4 position. Tetrachloroanisol, the Me ether of tetrachlorophenol, did not inhibit the reaction, and inhibition by 2,5-dichlorophenol, which has a pKa of 7.2, was pH dependent, suggesting that the anionic form of the phenol is the inhibitor. TCP inhibition of the carboxylase is not competitive vs. vitamin K in vitro, but that in vivo antagonism by TCP can be reversed with vitamin K. Rats given 40 mg/kg TCP had decreased plasma prothrombin levels and increased amts. of liver microsomal prothrombin precursors, whereas rats injected with 1 mg vitamin K 24 h before the TCP injection had normal levels of both. Vitamin K administration could not overcome completely the effects of 100 mg/kg TCP. Animals injected with TCP had increased levels of vitamin K 2,3-epoxide in the liver, which would be consistent with a partial inhibition of the microsomal vitamin K-epoxide reductase by this anticoagulant.

IT 25486-55-9, Vitamin K 2,3-epoxide

RL: BIOL (Biological study)

(of liver microsomes, tetrachloropyridinol effect on)

RN 25486-55-9 CAPLUS

CN Naphth[2,3-b]oxirene-2,7-dione, 1a,7a-dihydro-la-methyl-7a-(3,7,11,15-tetramethyl-2-hexadecen-1-yl)- (CA INDEX NAME)

L18 ANSWER 7 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1990:231749 CAPLUS

DN 112:231749

TI Substituted vitamin K epoxide analogs. New competitive inhibitors and substrates of vitamin K1 epoxide reductase

AU Ryall, Robert P.; Nandi, Dhirendra L.; Silverman, Richard B.

CS Dep. Chem., Northwestern Univ., Evanston, IL, 60208-3113, USA

SO Journal of Medicinal Chemistry (1990), 33(6), 1790-7 CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

Several 2- and 3-substituted vitamin K 2,3-epoxide analogs were AB synthesized and tested as inactivators, inhibitors, and substrates for bovine liver microsomal vitamin K1 epoxide reductase (I). 2-(X)-3-phytyl-1,4-naphthoquinone 2,3-epoxides, where X is hydroxymethyl, chloromethyl, fluoromethyl, difluoromethyl, and formyl were all competitive inhibitors, but none was an inactivator. Only the 2-hydroxymethyl analog was reduced to a quinone that was stable enough under the conditions of the experiment to be detected. Vitamin K1 epoxide analogs with modified phytyl chains (1'-hydroxy, 3'-fluoro with isomerized double bond, 1'-hydroxy and 1'-fluoro with saturated double bond, and the corresponding unsubstituted chains) were synthesized. All of the analogs were competitive inhibitors of I. The nonfluorinated analogs also were shown to be substrates, being reduced to the corresponding quinones without enzyme inactivation. At least one other enzyme besides I in bovine liver microsomes also metabolized all of these analogs.

IT 25486-55-9DP, Vitamin K1 epoxide, analogs

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and interaction with vitamin K epoxide reductase)

RN 25486-55-9 CAPLUS

CN

Naphth[2,3-b]oxirene-2,7-dione, la,7a-dihydro-la-methyl-7a-(3,7,11,15-tetramethyl-2-hexadecen-1-yl)- (CA INDEX NAME)

L18 ANSWER 8 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1988:200781 CAPLUS

DN 108:200781

TI Vitamin K-dependent carboxylase. Stoichiometry of vitamin K epoxide formation,  $\gamma$ -carboxyglutamyl formation, and  $\gamma$ -glutamyl-3H cleavage

AU Wood, Gary M.; Suttie, J. W.

CS Coll. Agric. Life Sci., Univ. Wisconsin-Madison, Madison, WI, 53706, USA

SO Journal of Biological Chemistry (1988), 263(7), 3234-9

CODEN: JBCHA3; ISSN: 0021-9258

DT Journal

LA English

Rat liver microsomal vitamin K-dependent carboxylase catalyzes the AB carboxylation of peptide-bound glutamyl (Glu) residues to γ-carboxyglutamyl (Gla) residues with the concomitant formation of vitamin K 2,3-epoxide (KO). These studies have demonstrated that the half-reaction, formation of KO, occurs in the absence of carboxylation at low glutamyl substrate concentration but that the ratio of KO-Gla approaches unity as the glutamyl substrate concentration is increased. Utilization of the carboxylase substrate Phe-Leu- $[\gamma-3H]$ Glu-Leu has demonstrated that the ratios of  $KO/\gamma$ -C-H bonds cleaved and  $Gla/\gamma$ -C-H bonds cleaved are equivalent at high substrate concns. and that these ratios approach unity. At low substrate concns., KO formation occurs at a higher rate than  $\gamma ext{-H}$  bond cleavage. These data are consistent with a mechanism involving the formation of an oxygenated intermediate from vitamin KH2 and O that is converted to KO during H abstraction from the  $\gamma$ -position of the Glu substrate. In the absence of a Glu substrate, the intermediate is converted to KO by a mechanism not coupled to glutamyl activation.

IT 25486-55-9, Vitamin K 2,3-epoxide

RL: FORM (Formation, nonpreparative)

(formation of, by vitamin K-dependent  $\gamma$ -glutamyl carboxylase,

stoichiometry and mechanism of)

RN 25486-55-9 CAPLUS

CN Naphth[2,3-b]oxirene-2,7-dione, 1a,7a-dihydro-1a-methyl-7a-(3,7,11,15-tetramethyl-2-hexadecen-1-yl)- (CA INDEX NAME)

ANSWER 9 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN L18

1987:12426 CAPLUS ΑN

DN 106:12426

Effect of N-methyl-thiotetrazole on vitamin K epoxide reductase ΤI

ΑU

Creedon, Kathleen A.; Suttie, J. W. Coll. Agric. Life Sci., Univ. Wisconsin, Madison, WI, 53706, USA CS

SO Thrombosis Research (1986), 44(2), 147-53

CODEN: THBRAA; ISSN: 0049-3848

DTJournal

English LA

AB Clin. use of antibiotics containing a N-methyl-thiotetrazole (NMTT) [13183-79-4] side chain has been reported to be associated with an increased incidence of a vitamin K [12001-79-5]-responsive hypoprothrombinemia. Administration of NMTT to rats decreased the activity of the liver microsomal vitamin K epoxide reductase [55963-40-1], increased the liver ratio of Vitamin K1 epoxide [25486-55-9] to vitamin K, and decreased the rate of metabolism of injected vitamin K epoxide. These responses are the same as those observed following the administration of coumarin anticoagulants. In contrast to the effect of coumarin anticoaqulants, NMTT did not inhibit the vitamin K epoxide reductase in vitro. These data suggest that the hypoprothrombinemia which has been observed following use of these antibiotics results from the inactivation of the liver vitamin K epoxide reductase by NMTT or a NMTT metabolite.

25486-55-9 ΙT

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(metabolism of, by liver, methylthiotetrazole effect on)

RN 25486-55-9 CAPLUS

Naphth[2,3-b]oxirene-2,7-dione, 1a,7a-dihydro-la-methyl-7a-(3,7,11,15-CN tetramethyl-2-hexadecen-1-yl)- (CA INDEX NAME)

ANSWER 10 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1986:454333 CAPLUS

105:54333

OREF 105:8761a,8764a

The vitamin K-antagonism of salicylate and warfarin

Roncaglioni, M. C.; Ulrich, M. M. W.; Muller, A. D.; Soute, B. A. M.; De ΑU Boer-Van den Berg, M. A. G.; Vermeer, C.

Dep. Biochem., Univ. Limburg, Maastricht, 6200 MD, Neth. CS

Thrombosis Research (1986), 42(6), 727-36 SO CODEN: THBRAA; ISSN: 0049-3848

DTJournal

LAEnglish

The effects of salicylate [69-72-7] and warfarin [81-81-2] on the plasma AB levels of coagulation factors and on the accumulation of endogenous substrates (e.g., clotting factor precursors) in liver and lung were examined in rats. When administered in high doses, salicylate acts as a vitamin K [12001-79-5]-antagonist; it induces a decrease of the plasma concentration of the Gla-containing coagulation factors and an accumulation of microsomal substrates for vitamin K-dependent carboxylase [9031-55-4] in

the liver and in the lung. In vitro, the drugs inhibit the DTT-dependent reductases which mediate the reduction, of vitamin K epoxide [ 25486-55-9] and vitamin K quinone [84-80-0]. NADH-dependent reductase [9037-80-3] and vitamin K-dependent carboxylase are not inhibited.

IT 25486-55-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(reduction of, reductase for, salicylate and warfarin effect on)

RN 25486-55-9 CAPLUS

CN Naphth[2,3-b]oxirene-2,7-dione, 1a,7a-dihydro-la-methyl-7a-(3,7,11,15-tetramethyl-2-hexadecen-1-yl)- (CA INDEX NAME)

L18 ANSWER 11 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1986:122492 CAPLUS

DN 104:122492

OREF 104:19175a,19178a

TI Quantitative analysis of pharmacological concentrations of vitamin K1 and vitamin K1 2,3-epoxide in rat liver by high-performance liquid chromatography

AU Cholerton, Suzanne; Park, B. Kevin

CS Univ. Liverpool, Liverpool, L69 2BX, UK

SO Journal of Chromatography (1986), 375(1), 147-53 CODEN: JOCRAM; ISSN: 0021-9673

DT Journal

LA English

GI

Liver vitamin Kl (I) [84-80-0] and vitamin Kl 2,3-epoxide (II) [ 25486-55-9] were determined following pharmacol. doses by normal-phase HPLC on Partisil 10 ODS with 0.23% MeCN in hexane as mobile phase for separation from interfering material followed by reversed-phase HPLC on Ultrasphere ODS Cl0 with 12.5% CH2Cl2 in MeCN as mobile phase. UV detection at 254 nm was performed. Recoveries were 61 and 77% for I and II, resp. The method was applied to study the response of liver I and II to anticoagulants.

IT 25486-55-9

RL: ANT (Analyte); ANST (Analytical study)
 (determination of, in liver by HPLC)

RN 25486-55-9 CAPLUS

CN Naphth[2,3-b]oxirene-2,7-dione, 1a,7a-dihydro-1a-methyl-7a-(3,7,11,15-

L18 ANSWER 12 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1985:499900 CAPLUS

DN 103:99900

OREF 103:15913a,15916a

TI Vitamin K epoxide reductase activity in the metabolism of epoxides

AU Liptay-Reuter, I.; Dose, K.; Guenthner, T.; Woerner, W.; Oesch, F.

CS Inst. Toxicol., Mainz, D-6500, Fed. Rep. Ger.

SO Biochemical Pharmacology (1985), 34(15), 2617-20

CODEN: BCPCA6; ISSN: 0006-2952

DT Journal

LA English

The importance of vitamin K epoxide reductase [55963-40-1] for the metabolism AB of a range of structurally diverse epoxides was investigated. Vitamin K1 epoxide [25486-55-9] is reduced by rat liver microsomes at a rate of 0.47 nmol/g liver/min. The rate of menadione oxide [15448-59-6] reduction is not significantly higher than the nonenzymic reduction rate. No measurable reduction of benzo[a]pyrene 4,5-oxide [37574-47-3], benzo[a]pyrene 7,8-oxide [36504-65-1], phenanthrene 9,10-oxide [585-08-0], styrene 7,8-oxide [96-09-3], and dieldrin [60-57-1] was detected, nor could T 2 toxin [21259-20-1] inhibit reduction of vitamin K1 epoxide. Thus, vitamin K epoxide reductase is very specific for vitamin K1 epoxide. Taking into account the range of structurally diverse epoxides investigated and the high specific activities of microsomal epoxide hydrolase [9048-63-9] and cytosolic glutathione transferase [50812-37-8] for these epoxides, it may be concluded that vitamin K epoxide reductase, in all likelihood, generally does not significantly contribute to the control of epoxides metabolically formed from xenobiotics.

IT 25486-55-9

RL: RCT (Reactant); RACT (Reactant or reagent) (reduction of, liver microsome vitamin K epoxide reductase effect on, epoxide metabolism in relation to)

RN 25486-55-9 CAPLUS

CN Naphth[2,3-b]oxirene-2,7-dione, 1a,7a-dihydro-1a-methyl-7a-(3,7,11,15-tetramethyl-2-hexadecen-1-yl)- (CA INDEX NAME)

AN 1985:418824 CAPLUS

DN 103:18824

OREF 103:3067a,3070a

Purification of a vitamin K epoxide reductase that catalyzes conversion of vitamin K 2,3-epoxide to 3-hydroxy-2-methyl-3-phytyl-2,3-dihydronaphthoguinone

AU Mukharji, Indrani; Silverman, Richard B.

CS Dep. Chem., Northwestern Univ., Evanston, IL, 60201, USA

Proceedings of the National Academy of Sciences of the United States of America (1985), 82(9), 2713-17 CODEN: PNASA6; ISSN: 0027-8424

DT Journal

LA English

An enzyme from bovine liver microsomes that catalyzes the reduction of vitamin AB K 2,3-epoxide to 2- and 3-hydroxy-2-methyl-3-phytyl-2,3dihydronaphthoquinone was purified 1152-fold to apparent homogeneity. Microsomes were solubilized with CHAPS and the enzyme was purified by chromatog. on PBE-94 ion exchanger, hydroxylapatite, and DEAE-cellulose, and then gel filtration on Sephacryl S-200. The homogeneity of the final preparation was established by SDS-polyacrylamide slab gel electrophoresis. The mol. weight of the native enzyme was 25,000 and that of the denatured enzyme was 12,400, suggesting that the enzyme is a dimer with identical subunits. No chromophoric cofactors were associated with the enzyme. Dithiothreitol and CHAPS were essential for activity, but high concns. of glycerol reduced the activity. The enzyme was not inhibited by Warfarin, a potent inhibitor of the vitamin K epoxide reductase which catalyzes the conversion of vitamin K 2,3-epoxide to vitamin K. Evidence is presented indicating that the purified enzyme is not simply a fragment of the Warfarin-sensitive vitamin K epoxide reductase.

IT 25486-55-9

RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with Warfarin-insensitive vitamin K epoxide reductase of liver microsomes)

RN 25486-55-9 CAPLUS

CN Naphth[2,3-b]oxirene-2,7-dione, 1a,7a-dihydro-1a-methyl-7a-(3,7,11,15-tetramethyl-2-hexadecen-1-yl)- (CA INDEX NAME)

L18 ANSWER 14 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1985:106109 CAPLUS

DN 102:106109

OREF 102:16523a,16526a

TI Indirect inhibition of vitamin K epoxide reduction by salicylate

AU Hildebrandt, E.; Suttie, J. W.

CS Coll. Agric. Life Sci., Univ. Wisconsin, Madison, WI, 53706, USA

SO Journal of Pharmacy and Pharmacology (1984), 36(9), 586-91 CODEN: JPPMAB; ISSN: 0022-3573

DT Journal

LA English

AB Salicylate [69-72-7] antagonizes the vitamin K [12001-79-5]-dependent biosynthesis of clotting factors in the rat and produces an elevation of the ratio of vitamin K epoxide [25486-55-9] to vitamin K in the

liver. Vitamin K epoxide is reduced to vitamin k by a vitamin K epoxide reductase [55963-40-1], and 1 mM salicylate was required to cause a 50% inhibition of the dithiothreitol-dependent in-vitro reduction of vitamin K epoxide by this enzyme. This enzyme was, however, inhibited 50% by as little as 70-80  $\mu\text{M}$  salicylate when reducing equivalent for the reaction were furnished by endogenous cytosolic reductants. This effect on the cytosolic reductant supply was shown to be unrelated to a previously demonstrated inhibition of DT-diaphorase by salicylate. The concns. of salicylate at which significant inhibitory effects are exerted are in-vitro (50-100  $\mu\text{M}$ ) are below the 200  $\mu\text{M}$  levels observed in the livers of rats given an anticoagulating dose of salicylate.

IT 25486-55-9

RL: BIOL (Biological study)

(of liver, salicylate effect on, clotting factor formation in relation to)

RN 25486-55-9 CAPLUS

CN Naphth[2,3-b]oxirene-2,7-dione, 1a,7a-dihydro-1a-methyl-7a-(3,7,11,15-tetramethyl-2-hexadecen-1-yl)- (CA INDEX NAME)

L18 ANSWER 15 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1984:468222 CAPLUS

DN 101:68222

OREF 101:10471a,10474a

TI Studies on vitamin K-dependent carboxylase from the cow

AU Vermeer, C.; Soute, B. A. M.; De Metz, M.

CS Dep. Biochem., State Univ. Limburg, Neth.

SO Posttransl. Covalent Modif. Proteins, [Int. Conf. Posttransl. Covalent Modif. Proteins Funct.] (1983), Meeting Date 1982, 231-51. Editor(s): Johnson, B. Connor. Publisher: Academic, New York, N. Y. CODEN: 51IFAP

DT Conference

LA English

AΒ The vitamin K (I)-dependent  $\gamma$ -glutamyl carboxylase (II) systems of human and bovine liver microsomes were compound Normal bovine liver microsomes contained extremely low amts. of endogenous carboxylatable substrate for II, whereas the human livers contained high amts. of this substrate(s). Sp-II (solid-phase II, prepared by extracting solubilized microsomes from Warfarin-treated cows with highly purified Sepharose-bound antifactor X antibodies) prepns. contained 40% phosphatidylcholine (PC) and a number of proteins (60%). PC was required for II activity, but its role was uncertain. Various organic solvents (e.g., ketones and DMSO) stimulated I-dependent II by 4-5-fold, but only when vitamin K1 forms, and not menadione derivs., were used as coenzyme. Apparently, these solvents interact with the I-binding site of II, facilitating I binding and mobility during the carboxylation reaction. This increased mobility in turn leads to a decrease in the activation energy of II, values which are quite high in the absence of the solvents (for the vitamin K1-driven reaction). All the data are consistent with a model in which the long phytyl side chain of vitamin K1 interacts strongly with a hydrophobic region of II, functioning only in carrying the reactive naphthoquinone group to the enzyme active site.

IT 25486-55-9

RL: BIOL (Biological study)

(vitamin K-dependent carboxylase of liver microsomes response to)

RN 25486-55-9 CAPLUS

CN Naphth[2,3-b]oxirene-2,7-dione, 1a,7a-dihydro-la-methyl-7a-(3,7,11,15-tetramethyl-2-hexadecen-1-yl)- (CA INDEX NAME)

L18 ANSWER 16 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1984:170517 CAPLUS

DN 100:170517

OREF 100:25869a,25872a

TI Relationship of dithiothreitol-dependent microsomal vitamin K quinone and vitamin K epoxide reductases. Inhibition of epoxide reduction by vitamin K quinone

AU Preusch, Peter C.; Suttie, John W.

CS Coll. Agric. Life Sci., Univ. Wisconsin, Madison, WI, 53706, USA

SO Biochimica et Biophysica Acta, General Subjects (1984), 798(1), 141-3 CODEN: BBGSB3; ISSN: 0304-4165

DT Journal

LA English

AB Vitamin K quinone was an effective inhibitor of vitamin K epoxide reduction by whole microsomes from rat liver. Inhibition was dependent upon the mode of addition of the substrate and inhibitor, suggesting segregation of the compds. into different microsomal vesicles under certain conditions. The result is consistent with reduction of both vitamin K quinone and vitamin K epoxide by a single enzyme or a multisite enzyme complex.

IT 25486-55-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(reduction of, by liver microsomes, vitamin K quinone inhibition of)

RN 25486-55-9 CAPLUS

CN Naphth[2,3-b]oxirene-2,7-dione, la,7a-dihydro-la-methyl-7a-(3,7,11,15-tetramethyl-2-hexadecen-1-yl)- (CA INDEX NAME)

L18 ANSWER 17 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1984:81749 CAPLUS

DN 100:81749

OREF 100:12339a,12342a

TI Solubilization and characterization of vitamin K epoxide reductase from

normal and Warfarin-resistant rat liver microsomes

AU Hildebrandt, E. F.; Preusch, P. C.; Patterson, J. L.; Suttie, J. W.

CS Coll. Agric. Life Sci., Univ. Wisconsin, Madison, WI, 53706, USA

SO Archives of Biochemistry and Biophysics (1984), 228(2), 480-92 CODEN: ABBIA4; ISSN: 0003-9861

DT Journal

LA English

Two procedures were developed for the solubilization of vitamin K epoxide ΑB reductase (I) from rat liver microsomal membranes by using the detergent Deriphat 160 at pH 10.8. The methods were applicable to both normal and Warfarin-resistant-strain rat liver microsomes and yielded material suitable for further purification The prepns. retained dithiothreitoldependent vitamin K quinone reductase activity as well as I and were free of vitamin K-dependent carboxylase and epoxidase activities. Optimal I activity was obtained at 0.1M KCl and pH 9 in the present of Na cholate. Artifactual formation of vitamin K metabolites was eliminated through the use of HgCl2 to remove excess dithiothreitol prior to extraction and metabolite assay. By using solubilized I, valid initial velocities were measured and reproducible kinetic data were obtained. The substrate initial velocity patterns were determined and were consistent with a ping-pong kinetic mechanism. The kinetic parameters obtained were a function of the cholate concentration, but did not vary drastically from those obtained with intact microsomal membranes. At 0.8% cholate, I solubilized from normal Warfarin-sensitive- and Warfarin-resistant-strain rat livers exhibited resp. values of Vmax = 3 and 0.75 nmol/min/g liver; Km for vitamin K epoxide = 9 and 4  $\mu$ M; and Km for dithiothreitol = 0.6 and 0.16 mM. IT 25486-55-9

RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with vitamin K epoxide reductase, kinetics of, Warfarin
 resistance in relation to)

RN 25486-55-9 CAPLUS

CN Naphth[2,3-b]oxirene-2,7-dione, 1a,7a-dihydro-la-methyl-7a-(3,7,11,15-tetramethyl-2-hexadecen-1-yl)- (CA INDEX NAME)

L18 ANSWER 18 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1983:590449 CAPLUS

DN 99:190449

OREF 99:29239a,29242a

TI Warfarin inhibition of vitamin K 2,3-epoxide reductase in rat liver microsomes

AU Fasco, Michael J.; Principe, Louise M.; Walsh, William A.; Friedman, Paul A.

CS Cent. Lab. Res., New York State Dep. Health, Albany, NY, USA

SO Biochemistry (1983), 22(24), 5655-60 CODEN: BICHAW; ISSN: 0006-2960

DT Journal

LA English

AB Warfarin (I) is a potent inhibitor of vitamin K 2,3-epoxide (II) reduction to vitamin K in vitro and in vivo. Dithiothreitol (DTT), an in vitro reductant for II reductase (III), antagonizes inhibition of III by I via mechanisms that have not yet been determined Expts. with rat hepatic

microsomes were undertaken to characterize the interactions that exist between I, II, and DTT. Increasing concns. of DTT decreased inhibition of III by I. When DTT was present prior to exposure of III to I, there was less inhibition than when the same concentration of DTT was present after its exposure to I. Moreover, maximum inhibition of III by I occurred at a much slower rate when DTT was present initially. Inhibition of III by I was greater when the substrate concentration was 100  $\mu\text{M}$  II than when it was 10  $\mu\text{M}$  II. On the basis of these data, it was concluded that (1) DTT reduces either directly or indirectly a critical disulfide bond within III that is reoxidized during reduction of II, (2) I and II are not competitive with respect to one another, and (3) I binding, which produces inhibition, occurs solely to the disulfide form of III. Once it is bound, I inhibits further reduction of the critical disulfide by DTT. DTT therefore antagonizes

by maintaining III in the reduced state.

IT 25486-55-9

Т

RL: BIOL (Biological study)

(vitamin K epoxide reductase of liver microsomes inhibition by Warfarin response to, in presence of dithiothreitol)

RN 25486-55-9 CAPLUS

CN Naphth[2,3-b]oxirene-2,7-dione, 1a,7a-dihydro-1a-methyl-7a-(3,7,11,15-tetramethyl-2-hexadecen-1-yl)- (CA INDEX NAME)

L18 ANSWER 19 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1983:175510 CAPLUS

DN 98:175510

OREF 98:26613a,26616a

TI Purification and properties of a factor from rat liver cytosol which stimulates vitamin K epoxide reductase

AU Siegfried, Charles M.

CS Med. Cent., Univ. Nebraska, Omaha, NE, 68105, USA

SO Archives of Biochemistry and Biophysics (1983), 223(1), 129-39 CODEN: ABBIA4; ISSN: 0003-9861

DT Journal

LA English

Two protein-type factors which stimulate the reduction of vitamin K1 AΒ 2,3-epoxide to vitamin K1 were separated from the 105,000 g supernatant fraction (cytosol) of rat liver homogenates. One of these factors was rather labile. However, the other factor was sufficiently stable to permit a 900-fold purification Four mg of this purified material were obtained in 32% yield from 11 g of soluble cytosolic protein. This factor appeared to be homogeneous, as determined by gel electrophoresis, and had a mol. weight of .apprx.38,000, as determined by gel filtration. The final preparation had no vitamin K epoxide reductase (I) activity in the presence or absence of either NADH or dithiothreitol. The results of kinetic studies using this factor were consistent with its acting as a nonessential activator of the microsome-catalyzed reduction of vitamin K1 2,3-epoxide. The factor did not cause a large change in the apparent Km of I (2.2-2.5  $\mu\text{M}$  in the absence and presence of activator, resp.), but the apparent Vmax was increased .apprx.4-fold.

IT 25486-55-9

RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with vitamin K epoxide reductase, kinetics of) 25486-55-9 CAPLUS

RN 25486-55-9 CAPLUS CN Naphth[2,3-b]oxirene-2,7-dione, 1a,7a-dihydro-1a-methyl-7a-(3,7,11,15-tetramethyl-2-hexadecen-1-yl)- (CA INDEX NAME)

L18 ANSWER 20 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1983:121904 CAPLUS

DN 98:121904

OREF 98:18517a,18520a

TI Stereospecificity of vitamin K-epoxide reductase

AU Preusch, Peter C.; Suttie, John W.

CS Coll. Agric. Life Sci., Univ. Wisconsin, Madison, WI, 53706, USA

SO Journal of Biological Chemistry (1983), 258(2), 714-16

CODEN: JBCHA3; ISSN: 0021-9258

DT Journal

LA English

The stereoselectivity of vitamin K-epoxide reductase (I) for the oxirane ring configuration of vitamin K epoxide (II) was determined by recovery of the partially resolved unreacted substrate following incubations of racemic II with rat liver microsomes. II was enriched for the (-)-enantiomer, but selectivity for the biol. relevant (+)-enantiomer was low. This result was confirmed by direct comparison of the rates of reaction for racemic II and (+)-II. The selectivity of I for the cis- or trans-phytyl configuration of the vitamin K side-chain was also low. These results suggest an enzyme active site which is open toward the 2,3-positions and is able to bind the substrate in 2 opposite orientations with respect to the positions of the Me and phytyl side-chain substituents.

IT 25486-55-9

RL: BIOL (Biological study)

(vitamin K epoxide reductase specificity for)

RN 25486-55-9 CAPLUS

CN Naphth[2,3-b]oxirene-2,7-dione, 1a,7a-dihydro-1a-methyl-7a-(3,7,11,15-tetramethyl-2-hexadecen-1-yl)- (CA INDEX NAME)

L18 ANSWER 21 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1982:99977 CAPLUS

DN 96:99977

OREF 96:16357a,16360a

TI Vitamin K epoxide reductase: evidence that vitamin K dihydroquinone is a product of vitamin K epoxide reduction

AU Sherman, Paula A.; Sander, Eugene G.

CS Dep. Biochem., West Virginia Univ., Morgantown, WV, 26506, USA

SO Biochemical and Biophysical Research Communications (1981), 103(3), 997-1005
CODEN: BBRCA9; ISSN: 0006-291X

DT Journal

LA English

AB Vitamin K epoxide reductase of rat liver is a 2-component enzyme system which catalyzes the reduction of vitamin K epoxide, using dithiothreitol as either a primary or secondary source of reducing equivalent A high-performance liquid chromatog. assay system indicates that in addition to the quinone, the dihydroquinone form of vitamin K is a reaction product. CM-cellulose chromatog. suggests that the same cytosolic protein fraction may be involved in the dithiothreitol-supported reduction of vitamin K epoxide, the dithiothreitol-supported reduction of vitamin K quinone, and the NADH-supported reduction of dichloroindophenol.

IT 25486-55-9

RL: RCT (Reactant); RACT (Reactant or reagent)
 (reduction of, by vitamin K epoxide reductase of liver)

RN 25486-55-9 CAPLUS

CN Naphth[2,3-b]oxirene-2,7-dione, 1a,7a-dihydro-1a-methyl-7a-(3,7,11,15-tetramethyl-2-hexadecen-1-yl)- (CA INDEX NAME)

L18 ANSWER 22 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1981:114409 CAPLUS

DN 94:114409

OREF 94:18551a,18554a

TI Age-dependent differences in the effect of phenprocoumon on the vitamin K1-epoxide cycle in rats

AU Trenk, Dietmar; Beermann, Dieter; Oesch, Franz; Jaehnchen, Eberhard

CS Pharmakol. Inst., Univ. Mainz, Mainz, D-6500, Fed. Rep. Ger.

SO Journal of Pharmacy and Pharmacology (1980), 32(12), 828-32 CODEN: JPPMAB; ISSN: 0022-3573

DT Journal

LA English

AB After phenprocoumon (I) [435-97-2] (0.355 mg/kg, i.v.) administration, the anticoagulant effect obtained was greater in older than in younger (36 and 12 wk, resp.) rats. The rate of elimination, volume of distribution, and the free fraction and free concentration values of I in plasma and liver

were

similar in older and younger rats. Following i.v. 3H-labeled vitamin K1 (II) [11104-38-4] ( $64.3~\mu g/kg$ ) and I (0.02-3~m g/kg), hepatic II-3H concentration decreased and 3H-labeled vitamin K1 2,3-epoxide (III) [25486-55-9] concentration increased in a dose- and hepatic I concentration-dependent manner. The changes were more pronounced in older than in younger rats; the concentration-response curves gave similar EC50 values for both age-groups, but a 1.6-fold higher maximum response, expressed as III/II ratios, in older rats. Thus, since anticoagulant drugs probably exert

their effect by inhibiting vitamin K1-epoxide reductase [55963-40-1], this enzyme may be more inhibited by I in older rats.

IT 25486-55-9

RL: BIOL (Biological study)

(cycle, phenprocoumon effect on, in aging)

RN 25486-55-9 CAPLUS

CN Naphth[2,3-b]oxirene-2,7-dione, 1a,7a-dihydro-1a-methyl-7a-(3,7,11,15-tetramethyl-2-hexadecen-1-yl)- (CA INDEX NAME)

L18 ANSWER 23 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1980:89866 CAPLUS

DN 92:89866

OREF 92:14671a,14674a

TI Studies of the vitamin K epoxide reductase system

AU Siegfried, Charles M.

CS Coll. Med., Univ. Nebraska, Omaha, NE, 68105, USA

SO Vitam. K Metab. Vitam. K-Dependent Proteins, [Proc. Steenbock Symp.], 8th (1980), Meeting Date 1979, 354-60. Editor(s): Suttie, John W. Publisher: Univ. Park Press, Baltimore, Md.

CODEN: 42IZAD

DT Conference

LA English

AΒ A protein (ERSA) was purified from liver cytosol which stimulated vitamin K epoxide reductase (I) activity and had no I activity itself. purification involved chromatog. on DEAE-Sephacel, quaternary aminoethyl-Sephadex, and Sephadex S-200. The step involving quaternary aminoethyl-Sephadex yielded 2 peaks; the major one comprised 87% of the activity, and only it was further purified. It stimulated I 4-5-fold, similar to the effect of the unpurified cytosol. Both vitamin K and vitamin K epoxide served equally well as effectors for vitamin K-dependent protein carboxylation. The rate of conversion of vitamin K epoxide to vitamin K in the vitamin K-dependent carboxylation system used was not sufficient to account for the amount of protein carboxylation observed Apparently, vitamin K and its epoxide may be converted to a common intermediate in their role in vitamin K-dependent carboxylation. The purified ERSA stimulated vitamin K-dependent protein carboxylation .apprx.2-fold.

IT 25486-55-9

RL: BIOL (Biological study)

(protein carboxylase stimulation by, vitamin K epoxide reductase activator protein effect on)

RN 25486-55-9 CAPLUS

CN Naphth[2,3-b]oxirene-2,7-dione, la,7a-dihydro-la-methyl-7a-(3,7,11,15-tetramethyl-2-hexadecen-1-yl)- (CA INDEX NAME)

L18 ANSWER 24 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1980:37038 CAPLUS

DN 92:37038 OREF 92:6163a

TI Determination of phylloquinone-2,3-epoxide and menaquinone-4-2,3-epoxide in biological materials by high performance liquid chromatography and fluorometric reaction detection

AU Hiroshima, Osamu; Abe, Kouichi; Ikenoya, Satoru; Ohmae, Masahiko; Kawabe, Kiyoshi

CS Anal. Res. Lab., Eisai Co., Ltd., Tokyo, Japan

SO Yakugaku Zasshi (1979), 99(10), 1007-13

CODEN: YKKZAJ; ISSN: 0031-6903

DT Journal

LA Japanese

Ahigh performance liquid chromatog. method was developed for the simultaneous determined of vitamin K and vitamin K oxide in biol. materials. The method involves n-hexane extraction of plasma or liver homogenate and reversed phase separation on Nucleosil C18 with a mobile phase of MeOH-EtOH (7:3) followed by fluorometric detection of the reaction products with NaHSO3-HCl and NaBH3CN. The min. detectable quantity was 2 ng for phylloquinone and menaquinone-4, and 3 ng for phylloquinone oxide and menaquinone-4 oxide. This method is simpler and more specific than the conventional methods for the determination of vitamin K oxide.

IT 25486-55-9

RL: ANT (Analyte); ANST (Analytical study)

(determination of, in biol. materials by high-performance liquid chromatog.)

RN 25486-55-9 CAPLUS

CN Naphth[2,3-b]oxirene-2,7-dione, 1a,7a-dihydro-1a-methyl-7a-(3,7,11,15-tetramethyl-2-hexadecen-1-yl)- (CA INDEX NAME)

L18 ANSWER 25 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1978:148032 CAPLUS

DN 88:148032

OREF 88:23283a,23286a

TI Enzymic hydroxymethylation of the benzene ring. 9. Activity of vitamin K in the enzymic hydroxymethylation of benzo $[\alpha]$ pyrene

AU Sloane, N. H.

CS Coll. Basic Med. Sci., Univ. Tennessee Cent. Health Sci., Memphis, TN, USA

SO Archives of Biochemistry and Biophysics (1978), 186(2), 401-5

CODEN: ABBIA4; ISSN: 0003-9861

DT Journal

LA English

AB Rat lung 6-hydroxymethylbenzo[a]pyrene synthetase was resolved into an apoenzyme by filtration of the holoenzyme through Amicon XM100 and XM50 filters. The enzymic activity was a function of the concentration of the lipid-soluble fraction prepared from the rat lung preparation when added to apoenzyme. The apoenzyme was purified ≥150-fold by these procedures. Vitamins K1 and K2, the 2,3-epoxide of vitamin K1, and menadione showed partial activity when substituted for the lung-lipid fractions. Some naphthoquinones also inhibited the reaction in the presence of vitamin K1. The synthetase reaction required NADPH.

IT 25486-55-9

RL: BIOL (Biological study)

(hydroxymethylbenzopyrene synthetase activation by)

RN 25486-55-9 CAPLUS

CN Naphth[2,3-b]oxirene-2,7-dione, 1a,7a-dihydro-la-methyl-7a-(3,7,11,15-tetramethyl-2-hexadecen-1-yl)- (CA INDEX NAME)

L18 ANSWER 26 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1977:529372 CAPLUS

DN 87:129372

OREF 87:20541a,20544a

TI Vitamin K epoxidase: properties and relationship to prothrombin synthesis

AU Sadowski, J. A.; Schnoes, H. K.; Suttie, J. W.

CS Coll. Agric. Life Sci., Univ. Wisconsin, Madison, WI, USA

SO Biochemistry (1977), 16(17), 3856-63

CODEN: BICHAW; ISSN: 0006-2960

DT Journal

LA English

ΑB

Postmitochondrial supernatants from vitamin K-deficient rat liver catalyze both the vitamin K-dependent conversion of microsomal precursor proteins to prothrombin, and the conversion of vitamin K1 to its 2,3-epoxide. Requirements for the latter reaction were studied, and the possible relation of the 2 reactions were investigated. The epoxidase activity was located in the microsomes and, if NAD(P)H was provided, no cytosolic component was required. The reduced pyridine nucleotides were needed to reduce vitamin K to its hydroquinone, and, when the hydroquinone was used as a substrate, no other source of reducing equivs. was required. The reaction required mol. O, which was incorporated into the epoxide. When the reaction was carried out in 2H2O, no 2H was incorporated into either the vitamin or its epoxide, suggesting that chromanol or methide forms of the vitamin were not intermediates in any of the reactions being studied. The epoxidn. of the vitamin was inhibited by direct antagonists of the vitamin, but not by the coumarin anticoagulant, warfarin. In general, conditions which favor epoxide formation also stimulate the formation of prothrombin. One major exception is the lack of dependence of epoxidn. on HCO3- concentration, but a requirement of HCO3- for prothrombin formation. data reported here are consistent with, but do not prove, the hypothesis that the epoxidn. reaction is coupled in some obligatory manner to the vitamin K-dependent carboxylation which is required for prothrombin

ľhe

formation. IT 25486-55-9

RL: BIOL (Biological study)

(prothrombin formation response to)

RN 25486-55-9 CAPLUS

CN Naphth[2,3-b]oxirene-2,7-dione, 1a,7a-dihydro-1a-methyl-7a-(3,7,11,15-tetramethyl-2-hexadecen-1-yl)- (CA INDEX NAME)

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L22 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN
     2004:633495 CAPLUS
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    141:151034
DN
TΙ
    Use of a composition comprising vitamin K1 oxide or a derivative
     thereof for the treatment and/or the prevention of mammalian
     dermatological lesions
ΙN
    Marchal, Alfred
PΑ
    Auriga International S.A., Belg.
SO
     PCT Int. Appl., 17 pp.
     CODEN: PIXXD2
DT
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L23 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN
    2004:633495 CAPLUS
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    141:151034
DN
    Use of a composition comprising vitamin K1 oxide or a derivative
ΤI
    thereof for the treatment and/or the prevention of mammalian
    dermatological lesions
ΙN
    Marchal, Alfred
    Auriga International S.A., Belg.
    PCT Int. Appl., 17 pp.
    CODEN: PIXXD2
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    Patent
    English
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L24 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2004:633495 CAPLUS

DN 141:151034

TI Use of a composition comprising vitamin K1 oxide or a derivative thereof for the treatment and/or the prevention of mammalian

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dermatological lesions
IN
     Marchal, Alfred
     Auriga International S.A., Belg.
PA
     PCT Int. Appl., 17 pp.
SO
     CODEN: PIXXD2
DT
     Patent
     English
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# PAGE 2-A

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L9 25 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN Naphth[2,3-b]oxirene-2,7-dione, la,7a-dihydro-la-(hydroxymethyl)-7a-

(3,7,11,15-tetramethyl-2-hexadecenyl) - (9CI)

MF C31 H46 O4

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

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L9 25 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN Naphth[2,3-b]oxirene-2,7-dione-1,2-1802, 1a,7a-dihydro-1a-methyl-7a-(3,7,11,15-tetramethyl-2-hexadecenyl)-, [7a(2E,7R,11R)]-[partial]- (9CI)

MF C31 H46 O3

Absolute stereochemistry.
Double bond geometry as shown.

$$\begin{array}{c|c} & \text{Me} & \text{Me} & \text{Me} \\ \hline & \text{CH}_2) & \text{R} & \text{CH}_2) & \text{R} & \text{CHMe}_2 \\ \hline & & \text{Me} & & \\ & & \text{Me} & & \\ \hline & & & \text{Me} & & \\ & & & & \text{CHMe}_2 \\ \hline & & & & & \\ \end{array}$$

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L9 25 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN Naphth[2,3-b]oxirene-2,7-dione-2-180, la,7a-dihydro-la-methyl-7a-(3,7,11,15-tetramethyl-2-hexadecenyl)-, (E)- (9CI)

MF C31 H46 O3

Double bond geometry as shown.

$$\begin{array}{c} \text{Me} \\ \text{CH2} \\ \text{Me} \\ \text{180} \end{array} \begin{array}{c} \text{Me} \\ \text{(CH2)} \\ \text{3} \end{array} \begin{array}{c} \text{Me} \\ \text{(CH2)} \\ \text{3} \end{array} \begin{array}{c} \text{CHMe2} \\ \text{CHMe2} \\ \text{Me} \\ \text{CHMe2} \end{array}$$

L9 25 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN Naphth[2,3-b]oxirene-la(2H)-carboxylic acid, 7,7a-dihydro-7a-(3-methyl-2-butenyl)-2,7-dioxo-, methyl ester (9CI)

MF C17 H16 O5

L9 25 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN Naphth[2,3-b]oxirene-2,7-dione, la-(chloromethyl)-la,7a-dihydro-7a-

(3,7,11,15-tetramethyl-2-hexadecenyl)- (9CI)

MF C31 H45 C1 O3

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L9 25 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN Naphth[2,3-b]oxirene-2,7-dione, 1a-[3,7,11,15,19,23-hexamethyl-25-(2,6,6-trimethyl-2-cyclohexen-1-yl)-2,10,14,18,22-pentacosapentaenyl]-1a,7a-dihydro-7a-methyl- (9CI)

MF C51 H74 O3

## PAGE 2-A

L9 25 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN Naphth[2,3-b]oxirene-2,7-dione, 1a,7a-dihydro-la-methyl-7a-(3,7,11,15-tetramethyl-2-hexadecenyl)-, [1aR-[1a $\alpha$ ,7a $\alpha$ (2E,7R\*,11R\*)]]- (9CI)

MF C31 H46 O3

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L9 25 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN Naphth[2,3-b]oxirene-2,7-dione, la,7a-dihydro-la-methyl-7a-(3-methyl-2-butenyl)-, (laS)- (9CI)

MF C16 H16 O3

Absolute stereochemistry.

L9 25 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN Naphth[2,3-b]oxirene-2,7-dione, 1a,7a-dihydro-la-methyl-7a-(3,7,11,15-

tetramethyl-2-hexadecenyl-1,2-t2)- (9CI)

MF C31 H44 O3 T2

L9 25 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN Naphth[2,3-b]oxirene-2,7-dione-1-180, la,7a-dihydro-la-methyl-7a-

(3,7,11,15-tetramethyl-2-hexadecenyl)-, [7a(2E,7R,11R)]-[partial]- (9CI)

MF C31 H46 O3

Absolute stereochemistry.
Double bond geometry as shown.

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IN Naphth[2,3-b]oxirene-2,7-dione-2-180, la,7a-dihydro-7a-methyl-la-(3,7,11,15-tetramethyl-2-hexadecenyl)-, (E)- (9CI)

MF C31 H46 O3

Double bond geometry as shown.

$$\begin{array}{c|c} & & & \\ &$$

L9 25 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN Naphth[2,3-b]oxirene-2,7-dione-1-180, 1a,7a-dihydro-1a-methyl-7a-

(3,7,11,15-tetramethyl-2-hexadecenyl)- (9CI) MF C31 H46 O3

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IN Naphth[2,3-b]oxirene-2,7-dione, la-(difluoromethyl)-la,7a-dihydro-7a-

(3,7,11,15-tetramethyl-2-hexadecenyl)-(9CI)

MF C31 H44 F2 O3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

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IN Naphth[2,3-b]oxirene-2,7-dione, la-(fluoromethyl)-la,7a-dihydro-7a-

(3,7,11,15-tetramethyl-2-hexadecenyl)- (9CI)

MF C31 H45 F O3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

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IN Naphth[2,3-b]oxirene-2,7-dione, la,7a-dihydro-la-methyl-7a-(3,7,11,15-tetramethyl-2-hexadecenyl)-, [laS-[la $\alpha$ ,7a $\alpha$ (2E,7S\*,11S\*)]]-

(9CI) MF C31 H46 O3

Absolute stereochemistry.
Double bond geometry as shown.

Me Me Me 
$$(CH_2)_3$$
 R  $(CH_2)_3$  CHMe2

R

Me  $(CH_2)_3$  R  $(CH_2)_3$  CHMe2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

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IN Naphth[2,3-b]oxirene-2,7-dione, la,7a-dihydro-la-methyl-7a-(3-methyl-2-butenyl)-, (laR)- (9CI)

MF C16 H16 O3

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

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IN Naphth[2,3-b]oxirene-2,7-dione, la,7a-dihydro-la-methyl-7a-(3,7,11trimethyl-2,6,10-dodecatrienyl)- (9CI)

MF C26 H32 O3

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IN Naphth [2,3-b] oxirene-2,7-dione, [1a,7a-dihydro-1a-methyl-7a-(3,7,11-dione)]

trimethyl-2-dodecenyl)- (9CI)

MF C26 H36 O3

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

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IN Naphth[2,3-b]oxirene-2,7-dione, la,7a-dihydro-la-methyl-7a-(3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22,26,30,34-

hexatriacontanonaenyl) - (9CI)

MF C56 H80 O3

PAGE 1-A

PAGE 1-C

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IN Naphth[2,3-b]oxirene-2,7-dione, la,7a-dihydro-la-methyl-7a-(3,7,10,13-tetramethyl-2-tetradecenyl)-, [laS-[la $\alpha$ ,7a $\alpha$ (2E,7S\*,10S\*)]]- (9CI)

MF C29 H42 O3

Absolute stereochemistry. Double bond geometry as shown.

$$\begin{array}{c|c}
 & Me \\
\hline
R & O \\
\hline
S & O \\
\hline
Me \\
\hline
Me \\
\hline
Me \\
\hline
Me
\end{array}$$
CHMe<sub>2</sub>

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L9 25 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN Naphth[2,3-b]oxirene-la(2H)-carboxaldehyde, 7,7a-dihydro-2,7-dioxo-7a-(3,7,11,15-tetramethyl-2-hexadecenyl)- (9CI)

MF C31 H44 O4

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

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IN Naphth[2,3-b]oxirene-2,7-dione, 1a,7a-dihydro-la-(hydroxymethyl)-7a-(3,7,11,15-tetramethyl-2-hexadecenyl)- (9CI)

MF C31 H46 O4

- L9 25 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
- IN Naphth[2,3-b]oxirene-2,7-dione, 1a-[3,7,11,15,19,23-hexamethyl-25-(2,6,6-trimethyl-2-cyclohexen-1-yl)-2,14,18,22-pentacosatetraenyl]-1a,7a-dihydro-7a-methyl- (9CI)
- MF C51 H76 O3

PAGE 1-A

PAGE 3-A

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Naphth[2,3-b]oxirene-2,7-dione, 1a,7a-dihydro-la-methyl-7a-(3-methyl-2-butenyl)- (9CI) C16 H16 O3

MF

0

O

Ме

L9 25 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN Naphth[2,3-b]oxirene-2,7-dione, 1a,7a-dihydro-1a-methyl-7a-(3,7,11,15-

tetramethyl-2,6,10,14-hexadecatetraenyl)-, (E,E,E)- (9CI)

MF C31 H40 O3

Double bond geometry as shown.

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

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IN Naphth[2,3-b]oxirene-2,7-dione, 1a,7a-dihydro-1a-methyl-7a-(3,7,11,15-1)

tetramethyl-2-hexadecen-1-yl)-

MF C31 H46 O3

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L11 STRUCTURE UPLOADED

=> d 111 L11 HAS NO ANSWERS L11 STR

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

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=> s 111 exa full FULL SEARCH INITIATED 20:06:51 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 1 TO ITERATE

100.0% PROCESSED 1 ITERATIONS 1 ANSWERS SEARCH TIME: 00.00.01

L12 1 SEA EXA FUL L11

=> d scan

L12 1 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN Naphth[2,3-b]oxirene-2,7-dione, 1a,7a-dihydro-1a-methyl-7a-(3,7,11-trimethyl-2,6,10-dodecatrienyl)- (9CI)

MF C26 H32 O3

### ALL ANSWERS HAVE BEEN SCANNED

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=> d l13 bib abs hitstr

L13 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1979:199712 CAPLUS

DN 90:199712

OREF 90:31714h,31715a

TI High-performance liquid chromatography of menaquinone-4, 2,3-epoxymenaquinone-4, demethylmenaquinone-4 and related compounds

AU Donnahey, Peter L.; Burt, Valerie T.; Rees, Huw H.; Pennock, John F.

CS Dep. Biochem., Univ. Liverpool, Liverpool, UK

SO Journal of Chromatography (1979), 170(1), 272-7 CODEN: JOCRAM; ISSN: 0021-9673

DT Journal

LA English

AB Thin-layer chromatog. (TLC) and high-performance liquid chromatog. (HPLC) were evaluated for use in the separation of the title vitamin K-related compds. Three TLC systems were tested: adsorption, on silica gel G with the solvent, 6% Et2O in light petroleum; argentation, on 10% AgNO3\*silica gel G with 60% diisopropyl ether in light petroleum; and reverse-phase, on

paraffin-impregnated Kieselguhr G with the solvent, 90% aqueous Me2CO. In addition, 3 HPLC systems were tested: (A) 3 + 30 cm µBondapak C18 column with acetonitrile-H2O (85:15) solvent; (B) 2 + 30 cm µBondapak C18 with MeOH solvent; and (C) 2 + 25 cm Partisil 10 ODS with acetonitrile-H2O (66:33) solvent. Since not all of the studied compds. could be separated clearly by a single TLC run, the HPLC system A was tested and found suitable for the separation of menadione, menaquinone-4 (and epoxy derivative), and menaquinone-3 (and epoxy derivative), whereas HPLC

was suitable for separation of phylloquinone and its epoxy derivative. The detection sensitivities for the HPLC and TLC systems were 5-10 and 250-500 ng, resp. HPLC system C was used to study the incorporation of mevalonic acid-2-14C into vitamin K in Carcinus maenas.

IT 70240-61-8

RL: ANT (Analyte); ANST (Analytical study)

(chromatog. of, high-performance liquid and thin-layer)

RN 70240-61-8 CAPLUS

CN Naphth[2,3-b]oxirene-2,7-dione, 1a,7a-dihydro-1a-methyl-7a-(3,7,11-trimethyl-2,6,10-dodecatrienyl)- (9CI) (CA INDEX NAME)

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L14 STRUCTURE UPLOADED

=> d 114

L14 HAS NO ANSWERS

L14

STR

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=> s exa full ENTER LOGIC EXPRESSION, QUERY NAME, OR (END):end SEARCH ENDED BY USER

=> s 114 exa full

FULL SEARCH INITIATED 20:11:34 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 19 TO ITERATE

100.0% PROCESSED 19 ITERATIONS

9 ANSWERS

SEARCH TIME: 00.00.01

L15 9 SEA EXA FUL L14

=> d scan

L15 9 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Naphth[2,3-b]oxirene-2,7-dione-1,2-1802, la,7a-dihydro-la-methyl-7a(3,7,11,15-tetramethyl-2-hexadecenyl)-, [7a(2E,7R,11R)]-[partial]- (9CI)
MF C31 H46 O3

Absolute stereochemistry. Double bond geometry as shown.

$$\begin{array}{c} \text{Me} \\ \text{E} \\ \text{CH2)} \\ \text{3} \end{array} \text{R} \begin{array}{c} \text{Me} \\ \text{(CH2)} \\ \text{3} \end{array} \text{CHMe2}$$

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L15 9 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Naphth[2,3-b]oxirene-2,7-dione-2-180, la,7a-dihydro-la-methyl-7a-(3,7,11,15-tetramethyl-2-hexadecenyl)-, (E)-(9CI)
MF C31 H46 O3

Double bond geometry as shown.

$$\begin{array}{c|c} & \text{Me} & \text{Me} & \text{Me} \\ \hline & \text{(CH2)} & \text{3} & \text{(CH2)} & \text{3} \end{array}$$

L15 9 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN Naphth[2,3-b]oxirene-2,7-dione, 1a,7a-dihydro-1a-methyl-7a-(3,7,11,15-tetramethyl-2-hexadecenyl)-, [1aS-[1a $\alpha$ ,7a $\alpha$ (2E,7S\*,11S\*)]]- (9CI)

MF C31 H46 O3

Absolute stereochemistry. Double bond geometry as shown.

$$\begin{array}{c} \text{Me} \\ \text{Me} \\ \text{CH}_2) \\ \text{3} \end{array} \begin{array}{c} \text{Me} \\ \text{(CH}_2) \\ \text{3} \end{array} \begin{array}{c} \text{CHMe}_2 \\ \text{CH}_2) \\ \text{Me} \end{array}$$

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IN Naphth[2,3-b]oxirene-2,7-dione, 1a,7a-dihydro-la-methyl-7a-(3,7,11,15-tetramethyl-2-hexadecenyl-1,2-t2)- (9CI)

MF C31 H44 O3 T2

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Absolute stereochemistry. Double bond geometry as shown.

L15 9 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Naphth[2,3-b]oxirene-2,7-dione-2-180, la,7a-dihydro-7a-methyl-la(3,7,11,15-tetramethyl-2-hexadecenyl)-, (E)- (9CI)
MF C31 H46 O3

Double bond geometry as shown.

$$\begin{array}{c|c} & & & \\ &$$

L15 9 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Naphth[2,3-b]oxirene-2,7-dione-1-180, 1a,7a-dihydro-1a-methyl-7a-(3,7,11,15-tetramethyl-2-hexadecenyl)-(9CI)
MF C31 H46 O3

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IN Naphth[2,3-b]oxirene-2,7-dione, 1a,7a-dihydro-1a-methyl-7a-(3,7,11,15-1)

tetramethyl-2-hexadecen-1-yl)-

MF C31 H46 O3

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

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